Gaussian Based Visualization of Gaussian and Non-Gaussian Based Clustering

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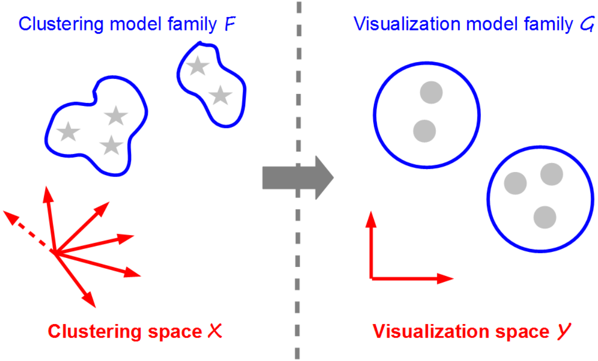
Take home message

Data/density visualization

Traditionally: chose the form of the mapping from $\mathcal{X}$ to $\mathcal{Y}$ for *user convenience*
Proposal: chose the form of the density of the data on $\mathcal{Y}$ for *cluster interpretation convenience*



Outline

Model-based clustering: pitch[1]

- Data set: $\mathbf{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$, each $\boldsymbol{x}_i \in \mathcal{X}$ with d_X variables (possibly mixing continuous, categorical, functional...)
- Unknown partition in K clusters : $\mathbf{z} = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n)$ with binary notation $\boldsymbol{z}_i = (z_{i1}, \ldots, z_{iK})$
- Statistical model: couples $(\boldsymbol{x}_i, \boldsymbol{z}_i)$ independently arise from the parametrized pdf

$$\underbrace{f(\boldsymbol{x}_i, \boldsymbol{z}_i)}_{\in \mathcal{F}} = \prod_{k=1}^{K} [\pi_k f_k(\boldsymbol{x}_i)]^{z_{ik}} \quad \Rightarrow \quad f(\boldsymbol{x}_i) = \sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x}_i)$$

- Estimating f: implement the MLE principle through an EM-like algorithm
- Estimating K: use some information criteria as BIC, ICL,...
- Estimating $\mathbf{z}$: use the MAP principle $\hat{z}_{ik} = 1$ iif $k = \arg\max_\ell t_{i\ell}(\hat{f})$ where

$$t_{ik}(f) = \mathrm{p}(z_{ik} = 1 | \boldsymbol{x}_i; f) = \frac{\pi_k f_k(\boldsymbol{x}_i)}{\underbrace{\sum_{\ell=1}^{K} \pi_\ell f_\ell(\boldsymbol{x}_i)}_{f(\boldsymbol{x}_i)}}.$$

[1] See for instance [McLachlan & Peel 2004], [Biernacki 2017]

Model-based clustering: poor user-friendly understanding

- n or K large: poor overview of partition $\hat{\mathbf{z}}$
- d_X large: too many parameters to embrace as a whole in $\hat{f}_k$
- Complex $\mathcal{X}$: specific and non trivial parameters involved in $\hat{f}_k$

Visualization procedures

Aim at proposing user-friendly understanding of the mathematical clustering results

Overview of clustering visualization: individual and pdf mappings

Indivdual mapping: visualize $\mathbf{x}$ and its estimated partition $\hat{\mathbf{z}}$

- Transforms $\mathbf{x}$, defined on $\mathcal{X}$, into $\mathbf{y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n)$, defined on a new space $\mathcal{Y}$

$$M^{\text{ind}} \in \mathcal{M}^{\text{ind}} : \ \mathbf{x} \in \mathcal{X}^n \mapsto \mathbf{y} = M^{\text{ind}}(\mathbf{x}) \in \mathcal{Y}^n$$

- Many methods, depending on $\mathcal{X}$ definition: PCA, MCA, MFA, FPCA, MDS. . .
- Some of them use $\hat{\mathbf{z}}$ in M^{ind}: LDA, mixture entropy preservation [Scrucca 2010]
- Nearly always, $\mathcal{Y} = \mathbb{R}^2$
- Model $\hat{f}(\boldsymbol{x}, \boldsymbol{z})$ is not taken into account, approach focused on $\mathbf{x}$

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Pdf mapping: display information relative to the f distribution

- Transforms $f = \sum_k \pi_k f_k \in \mathcal{F}$, into a new mixture $g = \sum_k \pi_k g_k \in \mathcal{G}$

$$M^{\text{pdf}} \in \mathcal{M}^{\text{pdf}} : \ f \in \mathcal{F} \mapsto g = M^{\text{pdf}}(f) \in \mathcal{G}$$

- $\mathcal{G}$ is a pdf family defined on the space $\mathcal{Y}$
- M^{pdf} is often obtained as a by product of M^{ind} (variable change formula)
- $\mathcal{G}$ is not a usual mixture family (Gaussian, ...) when M^{ind} is a nonlinear mapping
- For large n, M^{ind} finally displays M^{pdf}
- Often, both $\mathbf{y}$ and g are overlaid

Traditional visualization strategies and proposal

Traditional strategies: Controlling the mapping family $\mathcal{M}^{\text{pdf}}$ [2]

$$\underbrace{\mathcal{G}(\mathcal{M}^{\text{pdf}})}_{\text{uncontrolled}} = \left\{ g : g = M^{\text{pdf}}(f), f \in \mathcal{F}, M^{\text{pdf}} \in \underbrace{\mathcal{M}^{\text{pdf}}}_{\text{controlled}} \right\}$$

- Nature of $\mathcal{G}$ can dramatically depend on the choice of $\mathcal{M}^{\text{pdf}}$
- It can potentially lead to very different cluster shapes!
- Arguments for traditional $\mathcal{M}^{\text{pdf}}$: user-friendly, easy-to-compute
- Examples: linear mappings in all PCA-like methods

[2] Similar thinking with $\mathcal{M}^{\text{ind}}$

Traditional visualization strategies and proposal

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Proposed strategy: Controlling the pdf family $\mathcal{G}$

$$\underbrace{\mathcal{M}^{\text{pdf}}(\mathcal{G})}_{\text{uncontrolled}} = \left\{ M^{\text{pdf}} : g = M^{\text{pdf}}(f), f \in \mathcal{F}, g \in \underbrace{\mathcal{G}}_{\text{controlled}} \right\}$$

- It is the reversed situation where $\mathcal{G}$ is controlled instead of $\mathcal{M}^{\text{pdf}}$
- Offer opportunity to impose directly $\mathcal{G}$ to be a user-friendly mixture family
- Strategy $\mathcal{M}$ and Strategy $\mathcal{G}$ are both valid but Strategy $\mathcal{G}$ is rarely explored!

[2] Similar thinking with $\mathcal{M}^{\text{ind}}$

Outline

Spherical Gaussians as candidates

- Users are usually familiar with multivariate spherical Gaussians on $\mathcal{Y} = \mathbb{R}^{d_Y}$
- Thus a simple and "user-friendly" candidate g is a mixture of spherical Gaussians

$$g(\boldsymbol{y}; \boldsymbol{\mu}) = \sum_{k=1}^{K} \underbrace{\pi_k}_{\text{from } f} \phi_{d_Y}(\boldsymbol{y}; \underbrace{\boldsymbol{\mu}_k}_{?}, \boldsymbol{I})$$

where $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$ and $\phi_{d_Y}(.; \boldsymbol{\mu}_k, \boldsymbol{I})$ the pdf of the Gaussian distribution

- with expectation $\boldsymbol{\mu}_k = (\mu_{k1}, \ldots, \mu_{kd_Y}) \in \mathbb{R}^{d_Y}$
- with covariance matrix equal to identity $\boldsymbol{I}$

$g(\cdot; \boldsymbol{\mu})$ should be then linked with f in order to define a sensible $\mathcal{G}$

$$\mathcal{G} = \{g : g(\cdot; \boldsymbol{\mu}), \boldsymbol{\mu} \in \arg\min \delta(f, g(\cdot; \boldsymbol{\mu})), f \in \mathcal{F}\}$$

g as the "clustering twin" of f

Question: how to choose δ since generally $\mathcal{X} \neq \mathcal{Y}$?
Answer: in our clustering context, δ should measure the clustering ability difference

Kullback-Leibler divergence of clustering ability between both f and $g(\cdot;\boldsymbol{\mu})$[2]

$$\delta_{\mathrm{KL}}(f, g(\cdot;\boldsymbol{\mu})) = \int_{\mathcal{T}} \mathrm{p}_f(\boldsymbol{t}) \ln \frac{\mathrm{p}_f(\boldsymbol{t})}{\mathrm{p}_g(\boldsymbol{t};\boldsymbol{\mu})} d\boldsymbol{t}$$

where

- p_f: pdf of proba. of classification $\mathbf{t}(f) = (\boldsymbol{t}_i(f))_{i=1}^n$, with $\boldsymbol{t}_i(f) = (t_{ik}(f))_{k=1}^{K-1}$
- $\mathrm{p}_g(\cdot;\boldsymbol{\mu})$: pdf of proba. of classif. $\mathbf{t}(g) = (\boldsymbol{t}_i(g))_{i=1}^n$, with $\boldsymbol{t}_i(g) = (t_{ik}(g))_{k=1}^{K-1}$
- $\mathcal{T} = \{\boldsymbol{t} : \boldsymbol{t} = (t_1, \ldots, t_{K-1}), t_k > 0, \sum_k t_k = 1\}$

Thus, g should produce a distribution of the class membership posterior probabilities similar the one resulting of f.

[2] p_f is the reference measure

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- A natural requirement: $\mathrm{p}_g(\cdot;\boldsymbol{\mu})$ and g should be linked by a one-to-one mapping
- Currently not true since rotations and/or translations are possible
- It means: for one distribution f, there is a unique optimal distribution $g(\cdot;\boldsymbol{\mu})$
- Additional constraints on $g(\cdot;\boldsymbol{\mu})$: $d_Y = K-1$, $\boldsymbol{\mu}_K = \mathbf{0}$, $\mu_{kh} = 0$ $(h > k)$, $\mu_{kk} \geq 0$

[2] p_f is the reference measure

Estimating the Gaussian centers

- The Kullback-Leibler divergence δ_{KL} has generally no closed-form
- Estimate it by the following consistent (in S) Monte-Carlo expression

$$\hat{\delta}_{\text{KL}}(f, g(\cdot;\boldsymbol{\mu})) = \underbrace{\frac{1}{S}\sum_{s=1}^{S} \ln \mathrm{p}_g(\boldsymbol{t}^{(s)};\boldsymbol{\mu})}_{L(\boldsymbol{\mu};\mathbf{t})} + \text{cst}$$

  with S independent draws of conditional proba. $\mathbf{t} = (\boldsymbol{t}^{(1)}, \ldots, \boldsymbol{t}^{(S)})$ from p_f
- It is the normalized (observed-data) log-likelihood function of a mixture model
- But, by construction, all the conditional probabilities are fixed in this mixture
- Thus, just maximize the normalized complete-data log-likelihood $L_{\text{comp}}(\boldsymbol{\mu};\mathbf{t})$:
  - $K = 2$: this maximization is straightforward
  - $K > 2$: use a standard Quasi-Newton algorithm with different random initializations, for avoiding possible local optima

From a multivariate to a bivariate Gaussian mixture

- g is defined on $\mathbb{R}^{K-1}$ but it is more convenient to be on $\mathbb{R}^2$
- Just apply LDA on g to display this distribution on its most discriminative map
- It leads to the bivariate spherical Gaussian mixture $\tilde{g}$

$$\tilde{g}(\tilde{\boldsymbol{y}}; \tilde{\boldsymbol{\mu}}) = \sum_{k=1}^{K} \pi_k \phi_2(\tilde{\boldsymbol{y}}; \tilde{\boldsymbol{\mu}}_k, \boldsymbol{I}),$$

  where $\tilde{\boldsymbol{y}} \in \mathbb{R}^2$, $\tilde{\boldsymbol{\mu}} = (\tilde{\boldsymbol{\mu}}_1, \ldots, \tilde{\boldsymbol{\mu}}_K)$ and $\tilde{\boldsymbol{\mu}}_k \in \mathbb{R}^2$
- Use the % of inertia of LDA to measure the quality of the mapping from g to $\tilde{g}$

Remark

If $\mathcal{X} = \mathbb{R}^d$ and f is a Gaussian mixture with isotropic covariance matrices, then the proposed mapping is equivalent to applying a LDA to the centers of f

Overall accuracy of the mapping between f and $\tilde{g}$

Use the following difference between the normalized entropies of f and $\tilde{g}$

$$\delta_{\mathrm{E}}(f,\tilde{g}) = -\frac{1}{\ln K}\sum_{k=1}^{K}\left\{\int_{\mathcal{X}} t_k(\boldsymbol{x};f)\ln t_k(\boldsymbol{x};f)d\boldsymbol{x} - \int_{\mathbb{R}^2} t_k(\tilde{\boldsymbol{y}};\tilde{g})\ln t_k(\tilde{\boldsymbol{y}};\tilde{g})d\tilde{\boldsymbol{y}}\right\}$$

- Such a quantity can be easily estimated by empirical values
- Its meaning is particularly relevant:
  - $\delta_{\mathrm{E}}(f,\tilde{g}) \approx 0$: the component overlap conveyed by $\tilde{g}$ (over f) is accurate
  - $\delta_{\mathrm{E}}(f,\tilde{g}) \approx 1$: $\tilde{g}$ strongly underestimates the component overlap of f
  - $\delta_{\mathrm{E}}(f,\tilde{g}) \approx -1$: $\tilde{g}$ strongly overestimates the component overlap of f

$\delta_{\mathrm{E}}(f,\tilde{g})$ permits to evaluate the bias of the visualization

Drawing $\tilde{g}$

- Cluster centers: the locations of $\tilde{\boldsymbol{\mu}}_1, \dots, \tilde{\boldsymbol{\mu}}_K$ are materialized by vectors
- Cluster spread: the 95% confidence level displayed by a black border
- Cluster overlap: iso-probability curves of the MAP classification for different levels
- Mapping accuracy: $\delta_{\mathsf{E}}(f, \tilde{g})$ and also % of inertia by axis

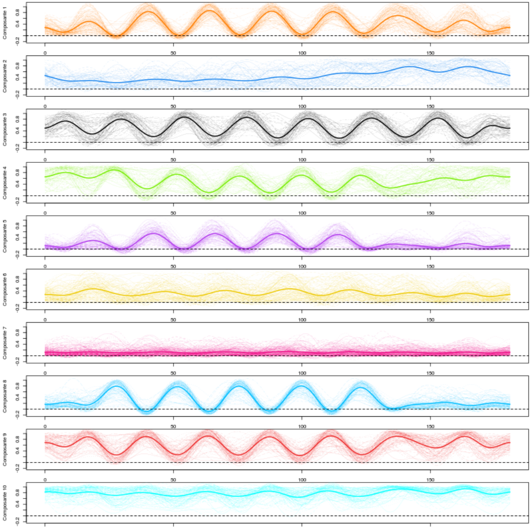
Outline

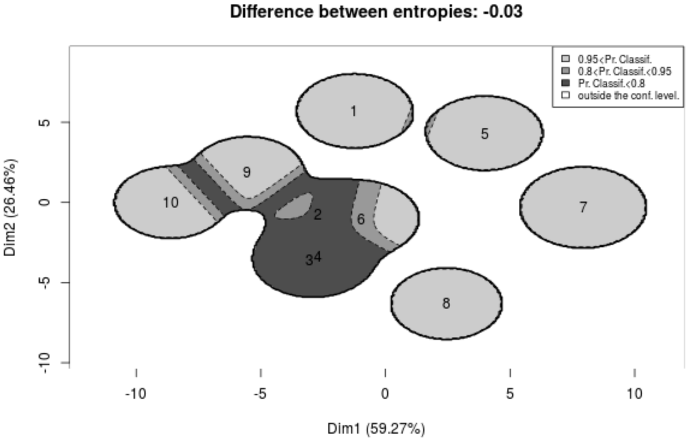
Bike sharing system: data[3] and model

- Station occupancy data collected over the course of one month on the bike sharing system in Paris
- Data collected over 5 weeks, between February, 24 and March, 30, 2014, on 1 189 bike stations
- Functional data: station status information (available bikes/docks) downloaded every hour from the open-data APIs of JCDecaux company
- The final data set contains 1 189 loading profiles, one per station, sampled at 1 448 time points
- Model: profiles of the stations were projected on a basis of 25 Fourier functions
- Model-based clustering of these functional data [Bouveyron *et al.* 2015] with the R package FunFEM [Bouveyron 2015]
- Retain 10 clusters
- Visualization using ClusVis R package

[3] [Bouveyron *et al.* (2015)]

Bike sharing system: cluster of curves visualization





Mapping of f on this graph is accurate because $\delta_{\mathsf{E}}(f, \tilde{g}) = -0.03$

Outline

Conclusion and extensions

Conclusion

- Generic method for visualizing the results of a model-based clustering
- Very easy to understand output since "Gaussian-like"
- Permits visualization for any type of data, because only based on proba. of classif.
- Can be used after any existing package of model-based clustering
- The overall accuracy of the visualization is also provided

Extensions

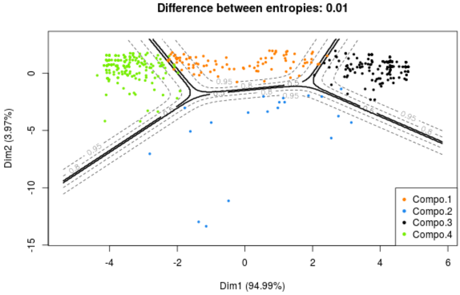
- Possibility to explore other pdf visualizations than Gaussians
- However, should keep in mind simple visualizations are targeted
- Possibility to compare pdf candidates through δ_{KL} or δ_{E}

About individual visualization

- Theoretically, impossible to obtain individual visualization from pdf visualization
- However, we can propose a pseudo scatter plot of $\mathbf{x}$ as follows

$$\boldsymbol{x}_i \longmapsto \boldsymbol{t}_i(f) = \boldsymbol{t}_i(g) \overset{\text{bijection}}{\longmapsto} \boldsymbol{y}_i \in \mathbb{R}^{K-1} \overset{\text{LDA}}{\longmapsto} \tilde{\boldsymbol{y}}_i \in \mathbb{R}^2$$

- $\tilde{\mathbf{y}}$ allows only to visualize the classification position of $\mathbf{x}$



- Caution: do not overlay pdf and individual plots since $\tilde{\mathbf{y}} = (\tilde{\boldsymbol{y}}_1, \ldots, \tilde{\boldsymbol{y}}_n)$ is not necessarily drawn from a Gaussian mixture

Model-based clustering: flexibility of $\mathcal{F}$ for complex $\mathcal{X}$

- Continuous data ($\mathcal{X} = \mathbb{R}^{d_X}$): multivariate Gaussian/t distrib. [McNicholas 2016]
- Categorical data: product of multinomial distributions [Goodman 1974]
- Mixing cont./cat.: product Gaussian/multinomial [Moustaki & Papageorgiou 2005]
- Functional data: the discriminative functional mixture [Bouveyron *et al.* 2015]
- Network data: the Erdös Rényi mixture [Zanghi *et al.* 2008]
- Other kinds of data, missing data, high dimension,. . .